

chain nodes :

7 8 9 10 11 12 13 14 21 22 23 24 25 26 27 28 34

ring nodes :

1 2 3 4 5 6 15 16 17 18 19 20

chain bonds :

2-13 4-7 4-8 6-9 9-10 10-11 10-12 12-34 13-14 16-27 18-21 18-22 20-23 23-24 24-25 24-26 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-12 12-34 13-14 15-16 15-20 16-17 17-18 18-19 19-20 24-25 24-26 27-28

exact bonds :

2-13 4-7 4-8 6-9 9-10 16-27 18-21 18-22 20-23 23-24

G1:C,CN,OH

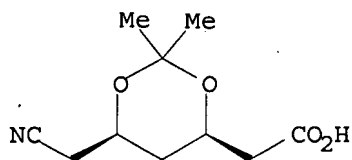
G2:H,Cs,Fr,K,Li,Na,Rb

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS12:CLASS13:CLASS14:CLASS15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS22:CLASS23:CLASS24:CLASS25:CLASS26:CLASS27:CLASS28:CLASS34:CLASS

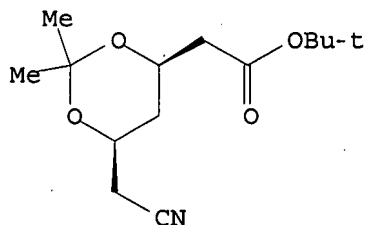
fragments assigned product role:

RX(11) OF 18 - 2 STEPS



- 1.1. PhMe
1.2. (COCl)₂
2.1. t-BuOH,
N-Methylmorpholine
2.2. PhMe

Na



REF: PCT Int. Appl., 2004096788, 11 Nov 2004

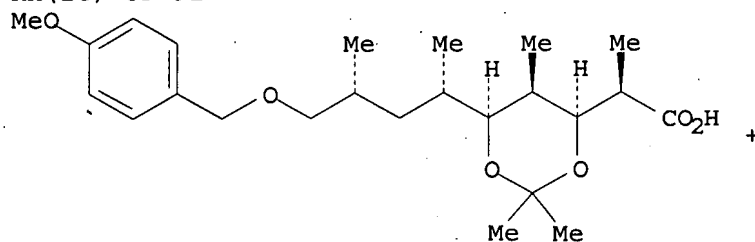
NOTE: 1) first stage Dean Stark app.

CON: STEP(1.1) room temperature
STEP(1.2) 2.5 hours, room temperature; 4 hours, room temperature
STEP(2.1) room temperature
STEP(2.2) 30 minutes, room temperature; 12 hours,
room temperature

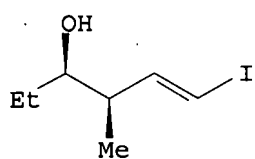
=>
=> d 1-23

L2 ANSWER 1 OF 23 CASREACT COPYRIGHT 2007 ACS on STN

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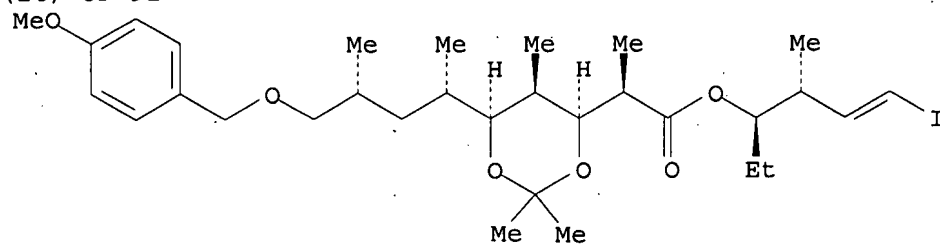
(step 1)



(step 2)

1. 2,4,6-Cl₃C₆H₂COCl,
Et₃N, THF
2. 4-DMAP, Benzene

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90%

REF: Journal of Organic Chemistry, 70(18), 7267-7272; 2005
CON: STAGE(1) 2 hours, room temperature
STAGE(2) 24 hours, room temperature